Запропоновано метод розв'язання задачі визначення невідомого складу газоподібного вуглеводневого палива в процесі його спалювання в режимі реального часу. Задача визначається як зворотна, некоректно поставлена. Спосіб виміру технологічних параметрів дозволяє її деталізувати як складну задачу інтерпретації.

Для вирішення цієї задачі обраний метод «бібліотеки» (підбору), який є найбільш універсальним. Для його реалізації розроблено метод формування бібліотеки у вигляді робочого тривимірного масиву. Вихідні дані для кожного рішення прямої задачі в сформованому масиві представлені у вигляді одного числа. Для цього використаний позиційний принцип запису десяткових чисел.

При формуванні робочого масиву використаний метод зіставлення коефіцієнта надлишку окиснювача і співвідношення об'ємних витрат окиснювача і пального. Це дозволило використовувати результати розв'язання прямої задачі визначення температури продуктів згоряння для розв'язання оберненої задачі по визначенню цього складу за виміряною температурою.

Розроблено метод пошуку рішення серед елементів робочого масиву на основі результатів технологічних вимірів температури продуктів згоряння палива, що спалюється і відношення об'ємних витрат окиснювача і пального.

Показано відсутність похибок, що вносяться до рішення алгоритмом пропонованого методу. При моделюванні точних технологічних вимірів похибки обумовлені дискретизацією вихідних даних при вирішенні прямої задачі. Визначено вплив точності вимірювань технологічних параметрів на похибку визначення складу пального. Вона не перевищує допустимої для інженерних розрахунків величини.

Запропонований метод розрахунку може дозволити використовувати в керованому режимі в енергетиці і в хімічній промисловості великий обсяг вуглеводневих горючих газів, які вважаються відходами. Їх енергетичний еквівалент порівняємо з енергетичними потребами Африканського континенту

Ключові слова: склад палива, зворотна задача, складне завдання інтерпретації, метод обмежень

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DETERMINING THE COMPOSITION OF BURNED GAS USING THE METHOD OF CONSTRAINTS AS A PROBLEM OF MODEL INTERPRETATION

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1. Introduction

The scientific, industrial, and business communities realize the urgent need to improve the energy efficiency of existing productions. This can reduce the share of energy resources in the cost of manufactured products and is one of the ways to improve their competitiveness. Thus, in many cases, improvement in energy efficiency is understood literally as reducing the consumption of energy resources per unit of output. In this case, enhancing energy efficiency necessitates improvement of technology in both energy generation and its utilization. That is associated with the need for substantial capital investment. The terms of implementation of such equipment are rather long.

Another way to bring down the cost of energy resources in the product cost is to consider a possibility to reduce the energy intensity of production. This could be achieved without energy efficiency improvements and significant financial expenditures, by lowering the cost of the consumed energy resources at existing energy equipment and with existing technologies. We are talking about different kinds of flammable substances, which form as a waste from existing types of industries or could be obtained when processing waste. One example is the gases produced in the coking, refinery production, blast furnace gases, products from mine degasification, associated gases from oil production, pyrolysis gases, gases from recycling, etc.

To use such energy resources in production, there should be a sufficient amount of them. Gases of different compositions must be collected in a single collector. And here is one of the tasks. The composition of the mixture is unknown and, moreover, it changes over time. That makes it difficult,

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or even exclude the very possibility, to use it without an operative determination of the composition. Thus, it is a relevant task to determine the composition of a gas mixture in real time.

2. Literature review and problem statement

One of the major constituent parts of associated gases is methane. At complete combustion of a certain volume of methane, an equivalent amount of carbon dioxide forms. According to the UN Intergovernmental Panel on Climate Change (IPCC) [1], the greenhouse activity of methane per 100 years is 28 times stronger than that for carbon dioxide of the same amount. Over a 20-year horizon, this magnitude is even larger – by 84 times. For this reason, in order to reduce environmental burdens, the associated gases that are not used for practical purposes are burnt in flare devices.

Based on estimates by the World Bank [2], in 2017, 141 billion cubic metres of gas were neutralized this way. According to [3], its rational use could have provided the African continent with electricity for one year. On the other hand, the cost of this gas may be about USD 30 billion dollars, which corresponds to a quarter of gas consumption in the United States, or to 30 % used in the European Union every year. In addition to burning, part of the gases is released directly into the atmosphere (degassing of mines, landfill gases, livestock waste, etc.). The data reported testify to the significance of the issue on rational use of associated gases. In additon to economic concerns, a big role belongs to environmental issues.

To date, there are several directions to manage the process of optimal flaring of gas of unknown composition.

Extreme regulators. For all their types, a common fault is predetermined by the very pattern of an extreme characteristic. Approaching an extremum point decreases (down to zero) the gradient of the measured parameter. This also applies to the case of determining the maximum temperature in a combustion chamber (furnace) [4], and to the case of determining the maximum temperature of a heat carrier [5]. The same property of the function is evident in determining the minimum (zero) concentration of carbon monoxide (CO) at minimum oxygen concentration in flue gases [6]. Given the existence of a sensititivity threshold and the errors in measurement systems, the point of extremum is exposed to the maximum errors in determining the desired signal. Noise in measuring channels also exerts a negative impact on the accuracy of determining a desired signal. As a consequence, the extremum point demonstrates the maximal measurement error.

The disadvantages greatly hinder, and in many cases exclude, a possibility to use extreme regulators while applying fuel of variable composition.

Gas analyzers. Another direction to ensure optimum parameters to manage the process of combustion or chemical conversion of hydrocarbon gases of unknown variable composition is to identify their components. In this scenario, there is a possibility to organize processes that do not possess extreme energy characteristics. One example is non-oxidative heating furnaces [8] or organic synthesis reactors.

When analyzing mixtures of gases in order to establish their qualitative and quantitative composition, one distinguishes chemical, physical-chemical, and physical methods. Significant advantages of the physical-chemical and physical methods over chemical, the speed of execution, a possibility to automate analysis, led to their more common application. Currently, the most widespread are methods of gas chromatography [9]. The main disadvantages of these devices is the consistent (not simultaneous) measurement of various components of gas, a long time of analysis, as well as the difficulties in detecting certain components.

Recently, researchers have discussed the design of gas analyzers based on using spontaneous Raman spectroscopy. With the advent of small, reliable laser sources and highly sensitive multichannel photodetectors the construction of such a tool has been considered in applied aspects [10], although it is, up to now, at the stage of labratory developments. In addition, these devices require a highly qualified service.

Determining the reduced formula of a mixture. Most calculations of the parameters for combustion processes (chemical conversion) are based on the methods of chemical kinetics for an individual substance [11]. The use of such an approach when considering the process of combustion of a gas mixture requires that its enthalpy and gross-formula should be defined. Paper [12] proposed a method for determining such a formula when burning the mixture used. Underlying it is the measurement of temperature of combustion products (CP) and the flow rate of an unknown gaseous fuel and air. It implies that the process of identifying the composition proceeds continuously in real time.

The stated problem is an inverse problem. Based on the measurements of technological parameters, the composition of a burned fuel is determined. Paper [12] shows that the solution to this problem does exist and it is unique. However, trying to find a solution has proven its instability. Thus, the stated problem, as is the case for most inverse problems, is ill-posed.

There is no a unified method to address the full diversity of inverse ill-posed problems. Each type requires an individual approach and includes an essential heuristic component. That complicates, or even rules out, the use of existing solving methods in an automated device for determining the gross formula of fuel of variable composition. In addition, the composition of fuel can repeatedly change within a small period of time. This implies the need for rapid multiple derivation of a solution for the problem. The result is the need to construct a new solving method.

3. The aim and objectives of the study

The aim of this study is to solve a problem on determining the composition of burned gas, using the method of constraints, as a problem on the interpretation of the model for determining the composition of burned fuel. This would make it possible to rationally utilize combustible gases and their mixtures of random and variable composition in terms of technological, energy, and environmental aspects.

To accomplish the aim, the following tasks have been set:

– to justify the choice of a method for solving the inverse ill-posed problem;

– to construct a technique to fill the library of solutions to a direct problem in the form of a three-dimensional array within the framework of chosen method for solving a complex interpretation problem as a kind of the inverse ill-posed problem;

– to devise a method to find a solution to the complex interpretation problem based on data from a working three-dimensional array;

– to determine the magnitude of error introduced to the solution when using the constructed method;

– to define the influence of error in the measurements of technological parameters on the accuracy of determining the composition of fuel.

4. The method of problem solving

4. 1. Substantiation of the choice of a solving method

Solving the inverse problem implies first of all a capability to solve the direct one.

When solving a direct problem, one of the original data sets is the oxidizer excess factor α. However, calculations employ a different quantity:

$$\chi = \alpha \cdot \chi_o, \tag{1}$$

where χ is the molar coefficient of components ratio; χ_0 is the molar stoichiometric coefficient of components ratio.

In any model, variables are divided into source data and calculation results. The group of source data includes those magnitudes whose *a priori* determination is possible. As regards the model under consideration, this is the oxidizer excess factor, determined only at a known composition of fuel and oxidizer. The results are partial pressures of substances in the mixture of CP and their temperature. Here, a certain possible direction for calculation emerges, thereby "detecting" a solution.

Let us make an assumption. We shall consider alternative types of fuel, which are in a gaseous state. When considering fuel and oxidizer as ideal gases, the magnitude χ can be defined based on the equality of molar volumes of any gases:

$$\chi = \dot{V}_{ox} / \dot{V}_f . \tag{2}$$

Here $\dot{V}_{ox}$ is the volumetric consumption of an oxidizing agent (air); $\dot{V}_f$ is the volumetric fuel flow rate. In other words, the magnitude χ (1) can be determined based on technological measurements of consumption without registering the chemical composition of the fuel and oxidizer. This property is applied to build a model for solving a problem on determining the composition of burned fuel based on the technological measurements of CP temperature and the volumetric consumption of fuel and oxidizer (an inverse problem).

When taking into consideration a series of factors, the need to "detect" a solution can be ruled out. These include limiting the predetermined list of chemical elements in the fuel gross-formula $C_{b_C}H_{b_H}O_{b_O}N_{b_N}$ [12]. In addition, it provides for the application of the measured magnitude of CP temperature T and the magnitude for a molar coefficient of components ratio χ in the form of a ratio of the measured volumetric consumption of oxidizer and fuel (2).

Next, the list of the magnitudes to be computed, along with the partial pressures of substances in CP, can be supplemented with one of the magnitudes for the number of atoms in the fuel gross-formula, for example, b_H. Its place in the source data is taken by the measured temperature of CP. We shall refer to this model as inverse in contrast to the original. Application of such an approach to describe other quantities, b_C, b_O, b_N, I_t – fuel enthalpy, makes it possible to record a model for determining the composition of fuel in the process of its combustion.

We assume that the composition of fuel remains constant over some time (opposing the violation of such a condition will be discussed below). This predetermines the invariability of values for the desired magnitudes b_C, b_H, b_O, b_N, I_t over the period of their determination. We assign a certain ratio of fuel and oxidizer with the measurement of their volumetric consumption ($\dot{V}_{ox}^1$ and $\dot{V}_f^1$). One measures the CP temperature T^1 when they are burned. These data underlie the recording of part of the model in the form of a set of equations (in the examined case – 13) that ensure determining 12 partial pressures P_j^1 and one of the desired magnitudes, for instance b_C. Next, we perform several changes to the ratio of volumetric consumption ($\dot{V}_{ox}^i$ and $\dot{V}_f^i$). For each of them, the CP temperature T^i is measured. The data obtained provide the basis for recording several more sets of equations needed to find the remaining desired magnitudes – b_H, b_O, b_N, I_t. In this case, one defines the corresponding number of sets of CP partial pressures P_j^i. Thus, in the examined case, the system of equations is written, consisting of 5 sets of 13 equations (total 65) to determine the 5 desired magnitudes and 5 groups of partial pressures. Each group corresponds to various ratios of volumetric consumption of fuel and oxidizer.

The scientific literature describes several techniques for solving a direct problem on determining the temperature of combustion products at known fuel composition. Many of them are used in solving particular variants. Paper [13] outlined the most universal approach. A solution is derived relative to the logarithms of the desired magnitudes. This makes it possible to smooth out the impact of a big difference (by 12–15 orders of magnitude) between partial pressures of substances in CP. Solving a system of nonlinear algebraic equations employs a Newton-Raphson method. Unsteadiness in a solution that occurs in some cases is overcome by introducing a lower relaxation coefficient not smaller than 0.5.

The system of equations derived in the manner described above is several times larger than those used in [13]. However, the equations used there are similar in the form. Attempting to apply the same approach to it when solving causes its instability under any conditions. An analysis showed that the cause of instability could be a bad conditionality in the system of linearized equations, obtained at solving. This is peculiar to inverse ill-posed problems, but is not mandatory.

To specify the reason for instability, a method from [13] was applied to solve a similar inverse problem described by a model of lesser dimensionality. The base was the above described 13 equations that can be used to determine any single desired magnitude, for example b_H. The result is the derived convergent solution under the same conditions as in [13]. Based on this, we can assume that the reason for instability is predetermined by not solving a given inverse problem.

The term "inverse problem" is often used to describe a "complex interpretation problem". One of its attributes is to measure a certain number of parameters independently of each other rather than simultaneously. This definition matches the problem under consideration and the model that describes it. To solve it, the most common, although cumbersome, is the method of a "library" (selection). Within its framework, the "filling" is carried out by repeatedly solving a direct problem at various combinations of source data. As a solution, one selects from a library of direct solutions an element that most closely matches the performed measurements. Such a solving process implies overcoming mathematical difficulties. As is the case for any ill-posed problems, a required element is the introduction of additional *a priori* information on the desired object and a solution. The success of solving it depends on the quality and quantity of information obtained from the experiment and on the technique of its processing. A non-classical solution involves modifying the representation of the model itself. In this case, the model includes both the *a priori* information on the possible character of the predicted solution, at least that reduces the informational uncertainty, and an information processing algorithm, that is, the derivation of a "solution". Based on these provisions, we have devised a method for solving the problem on determining the composition of fuel.

4. 2. A technique to fill a library of solutions to a direct problem in the form of a working three-dimensional array

The preparatory stage of defining a gross-formula for fuel, filling the library of solutions to a direct problem must involve the variation of 6 magnitudes. These include the possible number of atoms in relevant elements in the fuel gross-formula (b_C, b_H, b_O, b_N), the possible magnitude for an oxidizer excess factor α, and the possible magnitude for fuel enthalpy I_t.

The number of intervals can vary. For certainty, we accept 100, which will make it possible to monitor a change in each magnitude b_C, b_H, b_O, b_N, for example in the interval 0.05…4.95 at step 0.05, the magnitude α – in the range 0.025…2.5 at step 0.025. This will require $(100)^6=10^{12}$ solutions to a direct problem while registering all results. At this stage, it is possible to reducing the dimensionality of the problem.

Given that nitrogen (N) is introduced to the composition of fuel only from the air, the magnitude b_N is excluded from the list of variables, and it will quantitatively be determined through the oxidizer excess factor α. Next, in accordance with [14], the number of variables in the problem can be reduced through normalization. To organize the optimal, or broadly, controlled fuel combustion process, one does not even need to know its gross-formula. It would suffice to specify the ratio of the constituent atoms of chemical elements. For example, a stoichiometric process of ethane combustion (and any other substance) can be managed both based on its complete formula and at the normalized number of atoms:

$$2C_2H_6+7O_2=4CO_2+6H_2O$$

or

$$4C_1H_3+7O_2=4CO_2+6H_2O. \tag{3}$$

Here, normalization is performed based on number of carbon atoms. In a gross-formula, the number of atoms need not be integers. Normalization can be performed for any chemical element. In the problem under consideration, the normalization is based on carbon. The number of carbon atoms is constant and equals 1. In this case, the gross formula is defined as:

$$C_1H_{(b_H/b_C)}O_{(b_O/b_C)}N_{(b_N/b_C)} \text{ or } C_1H_{d_H}O_{d_O}N_{d_N}. \tag{4}$$

The result is the number of solutions to a direct problem decreases to $(100)^4=10^8$ implementations.

At the next stage, the presented method is used to convert the results obtained into a form that is convenient to use when finding a solution based on the performed technological measurements of CP temperature and the volumetric consumption of fuel and oxidizer:

1. A major proportion in the volume of calculation results when solving a direct problem is taken by the partial pressures of gases in a CP mixture. They do not take part in the process of determining the composition of starting fuel and are not reflected in the resulting library of solutions to a direct problem.

2. By varying d_H, d_O, d_N, (4) is used to assign a specific composition of fuel for each implementation of the solution to a direct problem. On this basis, one can define for each case a molar stoichiometric coefficient of components ratio χ_0. Considering (1), (2), a change in the magnitude for an oxidizer excess factor α is recalculated into a change in the ratio of the measured technological parameters $\dot{V}_{ox}/\dot{V}_f$.

3. With all possible combinations of source data $\dot{V}_{ox}/\dot{V}_f$ (α), d_H, d_O, d_N and I_t, resulting from varying their magnitudes, an attempt is made to solve the direct problem on determining the temperature of CP. In some cases, the considered ratio of fuel composition and its enthalpy is incompatible. Such variants of calculations are excluded from consideration.

4. For the remaining (successful) implementations of solution to a direct problem the set of source data d_H, d_O, d_N and I_t is written in the form of a single number based on the position principle for representing decimal numbers. To this end, the data are first recorded in the normalized form. For example:

$$\bar{d}_H=\frac{d_H-d_H^l}{d_H^r-d_H^l}\cdot 100. \tag{5}$$

Here, d_H is the number of hydrogen atoms in the considered implementation of a direct problem; d_H^l, d_H^r are the left and right boundaries of the considered interval of change in the magnitude for the number of hydrogen atoms when solving a direct problem. In the considered case, the multiplier "100" corresponds to the number of steps of change in d_{H}. Its magnitude is due only to the selected range (0…4.95) and the step (0.05) of change. The result is $\bar{d}_{\mathrm{H}}\in[00\ldots99]$. Similarly converted are d_O, d_N and I_t, thereby yielding respective magnitudes for $\bar{d}_O$, $\bar{d}_N$ and $\bar{I}_t$, whose values also change in the same or a similar interval. The obtained values are combined into a single number "*E*" by assigning them to appropriate bits (Fig. 1). For certainty, we assign the value $\bar{I}_t$ to its first bits. Note that the order to form this number can be any other. The result is the formed complexes, in which each pair of values for the results from solving a direct problem (*T* and $\dot{V}_{ox}/\dot{V}_f$) matches a single number with packaged values for their corresponding source data;

$$E_k=\boxed{\underbrace{1\,|\,2}_{I_t}\,|\,\underbrace{3\,|\,4}_{\bar{d}_H}\,|\,\underbrace{5\,|\,6}_{\bar{d}_O}\,|\,\underbrace{7\,|\,8}_{\bar{d}_N}}$$

Fig. 1. Schematic of positional representation of the normalized values for source data in the form of a single number

5. One structures the calculation results (*T* and $\dot{V}_{ox}/\dot{V}_f$). For this purpose, one defined their max [T^r, $(\dot{V}_{ox}/\dot{V}_f)^r$] and min [$T^l$, $(\dot{V}_{ox}/\dot{V}_f)^l$] values. The ranges of their change are divided into a certain number of intervals. The number of intervals and, respectively, the magnitude of step in the change of each magnitude correspond to the available technological

precision of magnitude measurements (T and $\dot V_{ox}/\dot V_f$) during fuel combustion.

6. By using the results from solving (T and $\dot V_{ox}/\dot V_f$) a direct problem and their corresponding source data, summarized in a single number "E", a three-dimensional array is built (Fig. 2). The plane $T-\dot V_{ox}/\dot V_f$ is split into cells with sides:

$$\Delta T=\frac{T^r-T^l}{N};\quad \Delta V=\frac{(\dot V_{ox}/\dot V_f)^r-(\dot V_{ox}/\dot V_f)^l}{M}. \tag{6}$$

Here, N, M is the number of elements (intervals) along the respective axes. The cells' borders are determined from ratios:

$$T_i^l=T^l+\Delta T\cdot(i-1);\quad T_i^r=T^r+\Delta T\cdot i;\quad i\in[0,N]; \tag{7}$$

$$(\dot V_{ox}/\dot V_f)_j^l=(\dot V_{ox}/\dot V_f)^l+\Delta V\cdot(j-1);$$

$$(\dot V_{ox}/\dot V_f)_j^r=(\dot V_{ox}/\dot V_f)^r+\Delta V\cdot j;\quad j\in[0,M], \tag{8}$$

where i, j are the numbers of cells along axes T и $\dot V_{ox}/\dot V_f$, respectively.

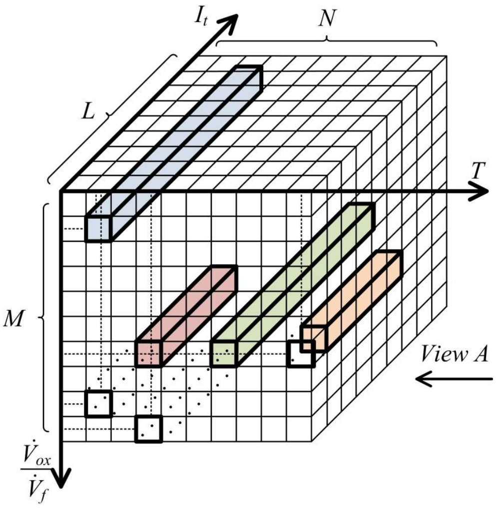

Fig. 2. Schematic of the formation of a structured working three-dimensional array based on source data and the results from solving a direct problem

7. Each cell is assigned with a vector of dimensionality (L) (Fig. 2) whose elements are the numbers "E". The magnitude for a number is determined from the value in the first (senior) bit. In the examined case, the values in the first bits are defined by the magnitude of enthalpy. Thus, the vectors axis is denoted as the axis of enthalpies I_t. A step in the change of magnitude for vector elements is determined in the same manner (6) applied for T or $\dot V_{ox}/\dot V_f$:

$$\Delta I_t=\frac{I_t^r-I_t^l}{L}, \tag{9}$$

and the range of change in enthalpies, corresponding to each element of the vector, is determined from ratios similar to (7) or (8):

$$(I_t^l)_k=I_t^l+\Delta I_t\cdot(k-1);\quad (I_t^r)_k=I_t^r+\Delta I_t\cdot k;\quad k\in[0,L]. \tag{10}$$

Here, I_t^l, I_t^r are the minimum and maximum values for enthalpies from the considered range of their change when solving a direct problem; ΔI_t is the step in enthalpy change; L is the number of elements into which one splits the examined range of enthalpy change. The magnitude L, similarly to M, N, is defined by a researcher considering the required precision in treating the respective magnitudes. Assume, for example, that in (6) $N=100$ and $M=100$. In this case, 10^4 cells form on plane $T-\dot V_{ox}/\dot V_f$. If the number of implementations of the solution to a direct problem is 10^8, each cell can be matched with the results from $\sim 10^8/10^4=10^4$ solutions. A similar quantity of numbers "E_k", associated with these solutions, are arranged inside the elements of respective vectors.

8. In the elements of the vector, one placed the values for "E_k", which are within their respective borders:

$$E_k\in[(I_t^l)_k,(I_t^r)_k]. \tag{11}$$

Some elements of the vectors remain unfilled because not all combinations of fuel composition ($\bar d_H$, $\bar d_O$, $\bar d_N$) can be implemented given the considered list of magnitudes for enthalpies I_t. The elements of the vectors are arranged in ascending order. Therefore, the values for numbers "E_k" within each vector are arranged in ascending order. Examples of populating certain vectors are shown in Fig. 2 marked with color.

Thus, based on solving preliminarily a set of direct problems and processing the calculation results, we have created a working three-dimensional array. Magnitudes from the array can be used when determining the composition of various fuels. It is important that their gross-formula should consist of the chemical elements used in forming the working array. In this case, some elements may not be available. For example, the examined array may serve as a basis for determining a composition of both oxygen-containing and oxygen-free hydrocarbons, when they burn in the air and in oxygen (without nitrogen).

4. 3. A method to find a solution to the complex interpretation problem based on the application of data from a working three-dimensional array

The method for determining fuel composition using the generated working three-dimensional array is implemented as follows:

1. By modifying and registering the magnitude for a ratio of volumetric consumption of fuel and oxidizer $(\dot V_{ox}/\dot V_f)_i$ one measures a CP temperature T_i for every case. The number of such changes and measurements is defined by the number of magnitudes to be determined. Thus, for the case of fuel of the type (4), one must define 4 magnitudes ($\bar d_H$, $\bar d_O$, $\bar d_N$, I_t) and, accordingly, perform 4 sets of measurements.

2. In accordance with these measurements, one finds 4 cells on plane $T-\dot V_{ox}/\dot V_f$ of the working three-dimensional array (marked with dashed lines in Fig. 2) and the associated vectors (highlighted). Data from the remaining vectors are not used at the current stage. Elements of the vectors are numbers E_k. Each vector in E_k contains the recorded all possible combinations of the determined magnitudes ($\bar d_H$, $\bar d_O$, $\bar d_N$, I_t), which provide for temperature T_i at $(\dot V_{ox}/\dot V_f)_i$ of the respective cell.

3. The selected vectors are mapped onto plane $\dot V_{ox}/\dot V_f-I_t$ (view A, Fig. 2), more precisely, onto axis I_t. Possible position of the vectors is shown in Fig. 3 and is highlighted.

4. At all ratios of change in the volumetric consumption, the composition and enthalpy of the determined fuel remain constant. Therefore, the corresponding magnitudes for num-

bers E_k must be the same in all the examined vectors. Given this, one selects such elements that are shown by region D in Fig. 3. In a real situation, this region can cover more than 2 intervals. All other elements in the considered vectors do not participate in subsequent transformations. The senior bits of numbers E_k reflect the values for fuel enthalpies. Therefore, in each interval (k–1↔k and k↔k+1), the elements of the vectors contain the sets of source data (numbers E_k) with identical enthalpies. More precisely, the enthalpies are in intervals $(I_t)_{k-1} \leftrightarrow (I_t)_k$ and $(I_t)_k \leftrightarrow (I_t)_{k+1}$, predetermined by the accuracy of their determination.

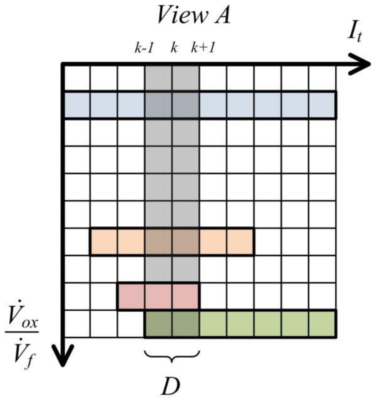

Fig. 3. Example of mapping the selected vectors

5. All the selected numbers (region D, Fig. 3) are rearranged in the stack order. The value from higher bits (Fig. 1) is moved to the end of the number. The higher bits accept the values for the next defined magnitude (Fig. 4).

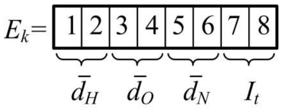

Fig. 4. Schematic of positional representation of the normalized values for source data after their rearrangement in the form of a single number

Within the range of the considered vectors, the remaining (rearranged) numbers are sorted, for example, in ascending order. The result is the scheme of position of the remaining numbers, similar to that shown in Fig. 3.

6. Steps from point 4 are repeated until one has used all the magnitudes from the list of the defined magnitudes (I_t, $\bar d_H$, $\bar d_O$, $\bar d_N$). In contrast to the first execution, one selects a number not with the same enthalpy I_t, but with a magnitude from higher bits of number E_k at the considered moment. Thus, during second run, it is $\bar d_H$, during third run – $\bar d_O$ and so on. Each iteration reduces the quantity of remaining numbers E_k. Ultimately, there remains one. It concentrates the source data corresponding to all measured T_i under assigned $\dot V_{ox}/\dot V_f$. This is the solution.

5. Examples of solving the problems on determining the composition of fuel

5. 1. Simulation of technological measurements without regard to instrumental errors

The efficiency of the proposed method was tested using an example of determining a preliminary known composition of methane (CH_4), propane (C_3H_8) and ethanol (C_2H_5OH). For methane, the rational, gross-formula, and the reduced gross formula are the same. For propane, the rational and gross-formula coincide. The reduced gross-formula takes the form $CH_{8/3}$ or $CH_{2,(6)}$. For alcohol, the gross-formula and the reduced formula take the form C_2H_6O and $CH_3O_{0,5}$, respectively. We have considered an example of burning these substances in oxygen. This makes it possible to use, in order to define the composition of fuel, a gross-formula of the following form:

$$CH_{\bar d_H} O_{\bar d_O}. \tag{12}$$

This choice, aimed at verifying the operability of our method, is due to the following reasons:

– using air as an oxidizer does not introduce to the combustion process any fundamental patterns compared with the use of oxygen. In this case, the absence of nitrogen makes the verification of operability of the method less cumbersome;

– the choice of alcohol as fuel is due to the presence of reference data [15] on the process of its combustion in oxygen (α, T, the CP composition). This ensures control over the validation of results from solving a direct problem when forming a working three-dimensional array;

– compliance with the requirement that the fuel should be in a gaseous state is provided for alcohol by considering the case of its being in the form of vapor and the corresponding enthalpy.

The original data in the form of technological measurements were simulated by the results from solving a direct problem for the respective substances. Two variants to assign the source data are considered:

1. Simulation of technological measurements without regard for instrument errors. The aim is to test the concept of the efficiency of the proposed method. Coincidence or deviation of the defined compositions of fuels from the assigned ones will determine the accuracy of the method's performance.

2. Simulation of technological measurements with a possible error of measurement. The aim is to assess the impact of a measurement error on the accuracy of determining the composition of the fuel.

The variant of assigning the source data does not affect the order of the formation of a working three-dimensional array. We accepted the following ranges of change in the original data:

– in (12):

$$\begin{aligned}
&\exists \bar d_H \in [0 \ldots 4{,}95]: \\
&(\bar d_H)_i = \Delta d \cdot (i-1), \\
&\Delta d = 0{,}05, \\
&\forall\, i \in [1 \ldots 100]; \\
&\exists \bar d_O \in [0 \ldots 4{,}95]: \\
&(\bar d_O)_i = \Delta d \cdot (i-1), \\
&\Delta d = 0{,}05, \\
&\forall\, i \in [1 \ldots 100].
\end{aligned} \tag{13}$$

– oxidizer excess factor α:

$$\exists\alpha\in[0{,}025\ldots2{,}5]:$$

$$\alpha_i=0{,}025+\Delta\alpha\cdot(j-1),$$

$$\Delta\alpha=0{,}025,$$

$$\forall\, j\in[1\ldots100]. \tag{14}$$

– fuel enthalpy I_t:

$$\exists I_t\in[-13500\ldots8800]\,\frac{\text{kJ}}{\text{kg}}:$$

$$(I_t)_i=-13500+\Delta I_t\cdot(i-1),$$

$$\Delta I_t=100,$$

$$\forall\, i\in[1\ldots224]. \tag{15}$$

The result is the derivation of $2.24\cdot10^8$ solutions to a direct problem. It took several hours for a common household personal computer. For all combinations of source data we calculated CP temperatures and recalculated the oxidizer excess factor α into the ratio of volumetric consumption of oxidizer and fuel $\dot{V}_{ox}/\dot{V}_f$. Part of the combinations of source data has proved to be incompatible. That was revealed in the course of solving a problem. After removing such combinations, a working array was formed. When using magnitudes in decimal form, its arrangement required ~2.7 Gb of memory. Upon converting to a binary form, the volume decreased to 1.2 Gb. The necessary resources could be found at all common PCs.

Using the proposed method for determining the composition of fuel has made it possible, for the examined substances (methane, propane, ethanol), to derive a solution that is precise within the framework of the model. The error is due to a sampling degree of the source data.

In the latter case, the presence of a range instead of a specific magnitude is explained, while the magnitude for an error is defined, by a data sampling step Δ*d* (13) when generating numbers E_k for a working three-dimensional array.

5. 2. Simulation of technological measurements with the imposed measurement error

The source data in the form of technological measurements were simulated by the results from solving a direct problem for methane and propane. We assigned different values for the oxidizer excess factor α, both larger and smaller than 1. We calculated the CP temperatures *T* for them and, based on (1), (2), the values for ratio $\dot{V}_{ox}/\dot{V}_f$. The obtained values, as is the case in a previous chapter, were taken as the "accurate" source data. Source data for solving the inverse problem on identification were obtained from the "accurate" ones by changing them in both directions by ±1 %. Solutions were sought under all possible combinations of the maximum deviation of source data from the "accurate" values.

During test "accurate" determining of the composition of methane, the found number of hydrogen atoms was always clearly equal to 4 or was defined by two magnitudes: 3.95 and 4. A range of ambiguity in the latter case is due to a sampling step (13) of this magnitude when solving a direct problem.

In the case under consideration, the solution is the ranges of possible values for the defined magnitudes. It is not always the case when there is a possibility to find a common range for all calculation variants. To improve the accuracy of a solution, we used an increased, compared to the theoretically required, number of measurements of technological parameters. We selected a range to serve as the solution (Fig. 3) with the highest number of matches among all the measurements of technological parameters. Thus, the solution is considered to be the most probable value for a defined magnitude.

The result of solving a problem is the obtained ranges of possible values for the number of hydrogen atoms in the normalized gross formulae and the oxidizer excess factor α when recording a stochiometric combustion reaction:

– for methane

$$\text{CH}_{3{,}7}\div\text{CH}_{4{,}1}\ \text{(precise value CH}_4\text{)}, \tag{16}$$

– for propane

$$\text{CH}_{2{,}5}\div\text{CH}_{2{,}75}\ \text{(precise value CH}_{2{,}(6)}\text{)}, \tag{17}$$

– for methane

$$\alpha\in[0{,}96\ldots1{,}01];\ \text{for propane}\ \alpha\in[0{,}98\ldots1{,}01]. \tag{18}$$

A range of change in α (18) was obtained by comparing the number of moles in oxygen in the corresponding stochiometric reaction under the boundary and accurate values for the number of hydrogen atoms in respective substances.

6. Discussion of results from solving a problem on determining the composition of burned gas by the method of constraints

The proposed solving method could be applied under a series of assumptions:

– the fuel whose composition is to be determined must be in a gaseous state;

– the properties of a gaseous fuel and the oxidizer obey the ideal gas equation;

– the composition of fuel during multiple technological measurements of CP temperature and its volumetric consumption should not change.

The first two assumptions are not strict for engineering calculations and are appropriate for any fuel composition. The method under consideration is proposed to be used when determining a variable composition of fuel. Therefore, the feasibility of the third assumptions must be considered further.

At the first stage, one must perform the required number of technological measurements to begin determining the fuel composition. For example, three sets of *T* and $\dot{V}_{ox}/\dot{V}_f$ {1, 2 and 3}. Based on them, one determines a first composition of the fuel. The following calculation necessitates a single measurement {4}; one can use the {2, 3, and 4} measurements as the source data. All further calculations are performed in the same sequence after a single ordinary measurement of a data set. In this case, after each calculation, the defined fuel composition is compared to the results from the previous step. The results that match testify to the absence of change in the composition of the fuel at the current step of measurements. Otherwise, one must discard the results from previous measurements. Perform three sets of measurements and calculate the new composition of fuel, similar to the first stage. Next steps follow the same pathway. Thus, one can detect the moment when the composition of the fuel changes.

Measuring the three data sets at the first stage of calculation is shown only as an example. The number of measurements can be any, based on necessity.

The volume of computational resources (external memory) and the time required for solving 10^8 variants of direct problems, utilized in forming a working three-dimensional array for a test problem, are significant (section 5.1). In this case, the composition of a gross formula of the fuel contained only three chemical elements: C, H and O. Adding each subsequent element increases in the avalanche fashion the number of solutions to a direct problem. One should consider the limits in applicability of the proposed solving method.

The gases whose composition is defined in most cases are organic compounds. Their composition can be defined by using six elements. In addition to the three mentioned above, one should take into consideration nitrogen (N), sulphur (S), phosphorus (P). All the source data that define the possible composition of a specific gas are represented in the form of a single number of the normalized values for source data (Fig. 1). Therefore, increasing the number of the considered chemical elements (from three to six) would increase the length of these numbers by two times only. When they are represented in a binary form, the required volume of external memory would also grow, but not exceeding 2.4 Gb.

The number of solutions to a direct problem would increase much larger. Assume that the range of possible number of atoms in the additionally introduced elements is similar to (13). A gross-formula of fuel that would account for each subsequent chemical element would increase the number of solutions by 100 times. In this case, the number of equations in the model also grows that prolongs the duration of individual solutions. When considering this issue, it should be taken into consideration:

– phosphorus (P) is rare in combustible gases and may be excluded from calculations without any significant effect;

– the amount of nitrogen (N) and sulphur (S) in a gross-formula of fuel is significantly smaller than the quantities of other included elements. The range of their possible change can be reduced compared to (13) while maintaining the same sampling step.

As a result, the number of solutions and, consequently, the time spent, would still significantly increase, but not as dramatically as it appeared originally.

Hardware also affects the rate of computation. Even common modern personal computers demonstrate the rate of calculations that is an order of magnitude larger than that used when solving a test problem. Moreover, solving a direct problem can run on multiple computers simultaneously. Fundamentally, this issue can be resolved by renting the operating time of a supercomputer in the Internet.

Solving the entire set of direct problems and filling the working array is performed once at the preliminary stage. In general, there are no limitations on time. Work can continue for 10 days and even 100 days.

The desired inverse problem is solved based on the generated working array when using a standard personal computer and it only takes a few seconds.

7. Conclusions

1. We have defined a general type of the problem as the inverse ill-posed problem and separated its narrower class of the complex interpretation problem. To solve it, we have chosen a library method (selection).

2. To fill the library, we devised a method for the structured and compact arrangement of results from solving direct problems. Within its framework:

– a method has been proposed to convert the oxidizer excess factor α as the source data for a direct problem in the ratio of volumetric consumption of oxidizer and fuel. The resulting magnitude is used as a measured technological parameter when solving the inverse problem on determining the fuel composition;

– a method has been suggested to convert the remaining source data in an direct problem (the number of atoms of chemical elements in a gross-formula and fuel enthalpy) into a single number, which is based on the principle of positional recording of decimal numbers.

3. We have devised a method to find a solution to the complex interpretation problem based on data from the generated working three-dimensional array by applying the constraints and by consistently selecting the regions where data converge. Such an approach makes it possible, at each step, to repeatedly reduce the volume of the analyzed quantities and, over a limited number of steps, to leave a single result that corresponds to the desired solution. This is the difference between the proposed method and the previously used method for direct sorting of data in a library.

4. The paper shows the absence of errors introduced to the solution by an algorithm of the proposed method. When modeling precise technological measurements, errors are attributable only to the source data sampling when solving a direct problem.

5. We have determined the influence of measurement accuracy of technological parameters on a measurement error in defining the composition of fuel. The magnitude of an error does not exceed the magnitude that is permissible for engineering calculations (<5 %).

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